

09/012,679

(FILE 'HOME' ENTERED AT 11:29:02 ON 15 APR 1999)

FILE 'REGISTRY' ENTERED AT 11:29:11 ON 15 APR 1999

L1 STRUCTURE UPLOADED  
L2 QUE L1  
L3 0 S L2  
L4 3 S L2 FULL

FILE 'CA' ENTERED AT 11:29:59 ON 15 APR 1999

L5 2 S L4

FILE 'REGISTRY' ENTERED AT 11:41:12 ON 15 APR 1999

L6 STRUCTURE UPLOADED  
L7 QUE L6  
L8 0 S L7  
L9 0 S L7 FULL  
E "BIS(CYCLOPENTADIENYL)TANTALUM TRIHYDRATE"/CN  
L10 1 S E2  
L11 STR 53522-50-2  
L12 0 S L11  
L13 25 S L11 FULL

FILE 'CA' ENTERED AT 11:53:29 ON 15 APR 1999

L14 0 S L12  
L15 78 S L13  
L16 0 S L15 AND CVD  
L17 74 S L15 AND PY<=1997  
L18 0 S L17 AND TANTALUM NITRIDE  
L19 0 S L17 AND TAN  
L20 0 S L17 AND TANTALUM AMIDE  
L21 0 S L17 AND TA FILM  
L22 0 S L17 AND TANTALUM FILM  
L23 1 S L17 AND CHEMICAL VAPOR DEPOSITION

=> s l13/p

L24 26 L13/P

=> d 1-26 bib abs

L24 ANSWER 1 OF 26 CA COPYRIGHT 1999 ACS

AN 129:16200 CA

TI On the Mechanism of Dihydrogen Addition to Tantalocene Complexes

AU Millar, Susan P.; Zubris, Deanna L.; Bercaw, John E.; Eisenberg, Richard  
CS Department of Chemistry, University of Rochester, Rochester, NY, 14627,  
USA

SO J. Am. Chem. Soc. (1998), 120(21), 5329-5330

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

AB The mechanism of addn. reaction of hydrogen to benzyne hydride  
tantalocene

complex to give trihydride complex, Cp\*TaH3 via intermediate dihydride  
complex, Cp\*TaH2, is described.

L24 ANSWER 2 OF 26 CA COPYRIGHT 1999 ACS

AN 127:135885 CA

TI Coordination behavior of LiBEt4 towards (.eta.5-C5H5)2ReH,

(.eta.5-C5H5)2WH2 and (.eta.5-C5H5)2TaH3. Solid state structure of

AU Fryzuk, Michael D.; Clentsmith, Guy K. B.; Rettig, Steven J.  
 CS Department of Chemistry, University of British Columbia, 2036 Main Mall,  
 Vancouver, BC, V6T 1Z1, Can.  
 SO Inorg. Chim. Acta (1997), 259(1-2), 51-59  
 CODEN: ICHAA3; ISSN: 0020-1693  
 PB Elsevier  
 DT Journal  
 LA English  
 AB The interactions of  $\text{LiBEt}_4$  with the early metal metallocene hydrides  
 $(\eta^5\text{-C}_5\text{H}_5)_2\text{M}^n\text{H}_n$  ( $\text{M} = \text{Ta}$ ,  $n = 3$ ;  $\text{M} = \text{W}$ ,  $n = 2$ ;  $\text{M} = \text{Re}$ ,  $n = 1$ ) were  
 studied. The 1:1 adduct formation between the Li cation of the sol. salt  
 and the hydride ligands of the neutral hydride complexes is quite stable  
 in soln.; competition expts. show that the strength of this interaction  
 increases as the no. of hydride ligands increases. The x-ray crystal  
 structure of  $[(\eta^5\text{-C}_5\text{H}_5)_2\text{TaH}.\text{cndot}.\text{AlH}_2(\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3)]_2$  is described; this is  
 the intermediate that forms when  $(\eta^5\text{-C}_5\text{H}_5)_2\text{TaCl}_2$  and  $\text{LiAlH}_4$  interact  
 in THF. The tetranuclear structure results from the bridging butoxy  
 groups which in turn arise from ring-opening of THF. Crystal data:  
 $[(\eta^5\text{-C}_5\text{H}_5)_2\text{TaH}.\text{cndot}.\text{AlH}_2(\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3)]_2$  ( $\text{C}_{28}\text{H}_{44}\text{Al}_2\text{O}_2\text{Ta}_2$ ),  
 monoclinic,  $a$  7.534(2),  $b$  11.433(1),  $c$  17.733(2) .ANG., .beta.  
 100.15(1).degree.,  $Z = 2$ , space group  $P2_1/c$ . The structure was solved by  
 Patterson methods and was refined by full-matrix least-squares procedures  
 to  $R = 0.036$  ( $R_w = 0.032$ ) for 1500 reflections with  $I \geq 3\sigma$ .  
 (I).

L24 ANSWER 3 OF 26 CA COPYRIGHT 1999 ACS  
 AN 127:109023 CA  
 TI Synthesis of and NMR T1 Relaxation in the Bimetallic Trihydride Complexes  
 $\text{Cp}_2\text{TaH}_2(\mu\text{-H})\text{M}(\text{CO})_5$  ( $\text{M} = \text{Cr}$ ,  $\text{Mo}$ ,  $\text{W}$ )  
 AU Bakmutov, Vladimir I.; Vorontsov, Evgenii V.; Boni, Gilles; Moise,  
 Claude  
 CS Institute of Organo-Element Compounds, Russian Academy of Sciences,  
 Moscow, 117813, Russia  
 SO Inorg. Chem. (1997), 36(18), 4055-4059  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB New bimetallic trihydrides  $\text{Cp}_2\text{TaH}_2(\mu\text{-H})\text{M}(\text{CO})_5$  [ $\text{M} = \text{Cr}$  (2),  $\text{Mo}$  (3),  $\text{W}$   
 (4)] were prepd. by the room-temp. high-yield reaction between  $\text{Cp}_2\text{TaH}_3$   
 (1) and  $\text{M}(\text{CO})_5$ . The complexes were characterized by elemental analyses and  
 variable-temp.  $^1\text{H}$  NMR and IR spectra. The structures and arrangements of  
 the hydride ligands in complexes 2-4, where the central hydride ligand is  
 bound to M, were detd. from  $^1\text{H}$  NMR and  $^1\text{H}$  T1 relaxation time data.  
 Structural interpretations of  $^1\text{H}$  T1 measurements, carried out for 1 and  
 bimetallic systems  $<295$  K, can be made from the isotropic motion approach  
 and of a model of uncoupled nuclei. The high-temp. satn. transfer expts.  
 in the  $^1\text{H}$  NMR spectra showed complexes 2-4 to be stereochem. nonrigid  
 demonstrating an HX/HA exchange on the T1 NMR time scale. The energy  
 barrier of the hydride/hydride exchange is decreased in going from  
 complex  
 1 to bimetallic systems 2-4.

L24 ANSWER 4 OF 26 CA COPYRIGHT 1999 ACS  
 AN 126:47310 CA  
 TI Exchange Coupling in Niobocene Trihydrides,  $\text{Nb}(\text{C}_5\text{H}_3\text{RR}')_2\text{H}_3$ , and Their  
 Adducts with Copper Triad Cations,  $[\{\text{Nb}(\text{C}_5\text{H}_3\text{RR}')_2\text{H}_3\}_2\text{M}]^+$  ( $\text{R} = \text{R}' = \text{H}$ ;  $\text{R} =$   
 $\text{H}$ ,  $\text{R}' = \text{SiMe}_3$ ;  $\text{R} = \text{R}' = \text{SiMe}_3$ ;  $\text{M} = \text{Cu}$ ,  $\text{Ag}$ ,  $\text{Au}$ )  
 AU Antinolo, Antonio; Carrillo-Hermosilla, Fernando; Chaudret, Bruno;  
 Fajardo, Mariano; Fernandez-Baeza, Juan; Lanfranchi, Maurizio; Limbach,  
 Hans-Heinrich; Maurer, Markus; Otero, Antonio; Pellinghelli, Maria Angela  
 CS Departamento de Quimica Inorganica, Universidad de Castilla-La Mancha,  
 Ciudad Real, 13071, Spain  
 SO Inorg. Chem. (1996), 35(26), 7873-7881  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB The reactions of  $\text{Nb}(\text{C}_5\text{H}_3\text{RR}')_2\text{Cl}_2$  with Red-Al followed by hydrolysis yield

$\text{Nb}(\text{C}_5\text{H}_3\text{RR}')_2\text{H}_3$  ( $\text{R} = \text{R}' = \text{H}$ , 1;  $\text{R} = \text{H}$ ,  $\text{R}' = \text{SiMe}_3$ , 2;  $\text{R} = \text{R}' = \text{SiMe}_3$ , 3). These compds. react with Lewis acidic coinage cationic species, namely,  $[\text{Cu}(\text{MeCN})_4]\text{PF}_6$ ,  $\text{AgBF}_4$ , and  $\text{Au}(\text{THT})\text{PF}_6$ , prepd. in situ from  $\text{AuCl}(\text{THT})$  and  $\text{TiPF}_6$  in a 2 to 1 ratio to yield  $[\{\text{Nb}(\text{C}_5\text{H}_3\text{RR}')_2\text{H}_3\}_2\text{M}]^+$  ( $\text{M} = \text{Cu}$ ,  $\text{R} = \text{R}' = \text{H}$ , 7;  $\text{R} = \text{H}$ ,  $\text{R}' = \text{SiMe}_3$ , 8;  $\text{R} = \text{R}' = \text{SiMe}_3$ , 9;  $\text{M} = \text{Ag}$ ,  $\text{R} = \text{H}$ ,  $\text{R}' = \text{SiMe}_3$ , 10;  $\text{R} = \text{R}' = \text{SiMe}_3$ , 11;  $\text{M} = \text{Au}$ ,  $\text{R} = \text{R}' = \text{H}$ , 12;  $\text{R} = \text{H}$ ,  $\text{R}' = \text{SiMe}_3$ , 13;  $\text{R} = \text{R}' = \text{SiMe}_3$ , 14). Like 1, but unlike the corresponding Ta derivs.  $\text{Ta}(\text{C}_5\text{H}_3\text{RR}')_2\text{H}_3$  ( $\text{R} = \text{R}' = \text{H}$ , 4;  $\text{R} = \text{H}$ ,  $\text{R}' = \text{SiMe}_3$ , 5;  $\text{R} = \text{R}' = \text{SiMe}_3$ , 6), and 3 show exchange couplings in their high-field  $^1\text{H}$  NMR spectra due to a hydride tunneling phenomenon. The magnitudes of exchange couplings are larger in the cases of 2 and 3 than in the case of 1 as a result of the decrease of electron d. upon increasing the no. of  $\text{SiMe}_3$  substituents on the Cp ring. The addn. of a Lewis acidic cation results in the observation of an AB2 pattern for the hydrides at room temp., which splits at low temp. into an ABC one in agreement with a fluxional behavior of the cation which binds to two hydrides of each Nb center. The activation energy of these fluxional processes are .apprx.42-45 kJ mol<sup>-1</sup> in the case of Cu adducts, 37 kJ mol<sup>-1</sup> in the case of Ag adducts, and 40 kJ mol<sup>-1</sup> in the case of Au adducts. The magnitude of exchange couplings is reduced upon addn. of Cu cation to 1-3, is of the same order of magnitude after addn. of a Ag cation, and is greatly increased by addn. of a Au cation.

A model is proposed to explain these variations which involves two isomeric states that are close in energy, one involving two bridging and one terminal hydrides on Nb and one involving one bridging hydride and a dihydrogen mol. A line shape anal. expt. carried out on 14 allows detn. of the parameters of the classical exchange, the coupling const. at various temps. which reach 550 Hz at 347 K, and the parameters of the quantum mech. exchange according to the authors' proposed model. The structure of 14 was studied by x-ray diffraction. The structure was solved from diffractometer data by Patterson method and refined by blocked full-matrix least squares from 3082 obsd. reflections to R and  $R_w$  values of 0.0346 and 0.0381, resp. The structure shows two bridging hydrides between the Nb and Au atoms; one of them is found close to the terminal hydride.

L24 ANSWER 5 OF 26 CA COPYRIGHT 1999 ACS  
 AN 125:168231 CA  
 TI Mixed-dicyclopentadienyl niobium and tantalum complexes: synthesis and reactivity. X-ray molecular structures of  $\text{Ta}(\eta^5\text{-C}_5\text{Me}_5)(\eta^5\text{-C}_5\text{H}_4\text{SiMe}_3)\text{Cl}_2$  and  $\text{Ta}(\eta^5\text{-C}_5\text{Me}_5)\{\eta^5\text{-C}_5\text{H}_3(\text{SiMe}_3)_2\}\text{H}_3$   
 AU Castro, Aurora; Gomez, Manuel; Gomez-Sal, Pilar; Manzanero, Antonio; Royo, Pascual  
 CS Departamento de Quimica Inorganica, Universidad de Alcala de Henares, Campus Universitario, Alcala de Henares, 28871, Spain  
 SO J. Organomet. Chem. (1996), 518(1-2), 37-46  
 CODEN: JORCAI; ISSN: 0022-328X  
 DT Journal  
 LA English  
 AB  $\text{MCP}^*\text{Cl}_4$  ( $\text{Cp}^* = \eta^5\text{-C}_5\text{Me}_5$ ) reacts with  $\text{LiCp}$  [ $\text{Cp} = \text{C}_5\text{H}_4(\text{SiMe}_3)$  ( $\text{Cp}'$ );  $\text{C}_5\text{H}_3(\text{SiMe}_3)_2$  ( $\text{Cp}''$ )] and sodium amalgam in 1:1:1 molar ratio to give the paramagnetic dicyclopentadienyl niobium and tantalum(IV) complexes  $\text{MCP}^*\text{CpCl}_2$  ( $\text{M} = \text{Nb}$ ,  $\text{Cp} = \text{Cp}'$  1;  $\text{Cp}''$  2;  $\text{M} = \text{Ta}$ ,  $\text{Cp} = \text{Cp}'$  3;  $\text{Cp}''$  4). Reactions of 3 and 4 with 1/2 equiv of  $\text{PCl}_5$  afford the diamagnetic trichloro complexes  $\text{TaCp}^*\text{CpCl}_3$  ( $\text{Cp} = \text{Cp}'$  5;  $\text{Cp}''$  6), while oxidn. with dry  $\text{O}_2$  gives the diamagnetic dinuclear complexes  $[\text{TaCp}^*\text{CpCl}_2]_2(\mu\text{-O})$  ( $\text{Cp} = \text{Cp}'$  7;  $\text{Cp}''$  8), and with air are transformed into the corresponding oxo derivs.  $\text{TaCp}^*\text{CpCl}(\text{O})$  ( $\text{Cp} = \text{Cp}'$  9;  $\text{Cp}''$  10). Treatment of compds. 3 and 4 with a slight excess of  $\text{LiAlH}_4$  affords the trihydrido complexes  $\text{TaCp}^*\text{CpH}_3$  ( $\text{Cp} = \text{Cp}'$  11;  $\text{Cp}''$  12). The trihydrido complex 12 reacts with two-electron donor ligands on heating to yield the hydrido tantalum(III) compds.  $\text{TaCp}^*\text{Cp}''\text{H}(\text{L})$  ( $\text{L} = \text{CO}$ ,  $\text{C}_2\text{H}_4$ ,  $\text{RNC}$ ). All the new complexes were characterized by usual IR and NMR spectroscopic methods. The crystal structures of 3 and 12 were detd. by x-ray diffraction studies. Crystals

of 3 are orthorhombic, space group P212121, with Z = 4 in a unit cell of dimensions a = 11.775(5) .ANG., b = 12.821(1) .ANG., c = 13.037(7) .ANG.. Crystals of 12 are triclinic, space group P.hivin.1 with Z = 2 in a unit cell of dimensions a = 7.384(4) .ANG., b = 10.861(2) .ANG., c = 16.731(3) .ANG., .alpha. = 75.94(2).degree., .beta. = 84.75(3).degree. and .gamma.

= 72.57(4).degree.. Both structures were solved from diffractometer data by a combination of direct and Fourier methods and refined by full-matrix least squares fit on the basis of 4088 (3) and 4594 (12) obsd. reflections to R and Rw values of 0.040 and 0.064 (3) and 0.022 and 0.033 (12) resp.

L24 ANSWER 6 OF 26 CA COPYRIGHT 1999 ACS

AN 125:33791 CA

TI Stereochemistry in Group 5 organometallic complexes: a metallocphosphine with an asymmetric tantalum center as precursor of chiral bimetallic derivatives

AU Sauvageot, Philippe; Moiese, Claude

CS Lab. synthese d'electrosynthese organometalliques, Faculte sciences

Gabriel, Dijon, 21000, Fr.

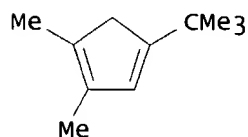
SO Bull. Soc. Chim. Fr. (1996), 133(2), 177-182

CODEN: BSCFAS; ISSN: 0037-8968

DT Journal

LA English

GI



I

AB A trisubstituted cyclopentadiene deriv. I was synthesized and used as a cyclopentadienyl ligand to obtain the Ta (IV) deriv. Cp'CpTaCl2.

Starting

from this dichloride, a multistep transformation (redn., carbonylation

and

reaction with  $\text{PMe}_2\text{Cl}$ ) leads to the chiral metallocphosphine  $\text{Cp}'\text{CpTa}(\text{CO})\text{PMe}_2$ , which contains an asym. Ta center. This metalloligand reacts with a carbonyl Cr fragment giving a chiral bimetallic deriv.  $\text{Cp}'\text{CpTa}(\text{CO})\text{PMe}_2\text{Cr}(\text{CO})_5$ .

L24 ANSWER 7 OF 26 CA COPYRIGHT 1999 ACS

AN 124:232678 CA

TI Convenient synthesis of  $\text{Cp}_2\text{TaH}_3$  using  $\text{LiAlH}_4$

AU Zvukova, T. M.; Sizov, A. I.

CS Department of Chemistry, M. V. Lomonosov State University, Moscow,

119899,

Russia

SO Izv. Akad. Nauk, Ser. Khim. (1995), (10), 2050-1

CODEN: IASKEA

DT Journal

LA Russian

OS CASREACT 124:232678

AB The prepn. of  $\text{Cp}_2\text{TaH}_3$  via the reaction between  $\text{TaCl}_5$ ,  $\text{CpNa}$ , and  $\text{LiAlH}_4$  in dimethoxyethane is described. The yield of  $\text{Cp}_2\text{TaH}_3$  is 25%.

L24 ANSWER 8 OF 26 CA COPYRIGHT 1999 ACS

AN 113:132367 CA

TI Copper(I) complexes with metal-metal (d10-d10) bond. Crystal and molecular structures of adducts of tantalocene trihydride with copper(I) iodide of composition:  $(\eta^5\text{-C}_5\text{H}_5)_2\text{TaH}[(\mu_2\text{-H})\text{Cu}(\mu_2\text{-I})_2\text{Cu}(\mu_2\text{-H})]_2\text{HTa}(\eta^5\text{-C}_5\text{H}_5)_2$ ,  $(\eta^5\text{-C}_5\text{H}_4\text{Bu-tert})_2\text{TaH}(\mu_2\text{-H})_2\text{Cu}(\mu_2\text{-I})_2\text{Cu}(\mu_2\text{-H})_2\text{HTa}(\eta^5\text{-C}_5\text{H}_4\text{Bu-tert})_2$ .  $\text{CH}_3\text{CN}$  and  $\{\text{Cu}(\mu_3\text{-I})\}_4\text{P}[\text{N}(\text{CH}_3)_2]_3$

AU Arkhireeva, T. M.; Bulychev, B. M.; Sizov, A. I.; Sokolova, T. A.; Bel'skii, V. K.; Soloveichik, G. L.

CS Dep. Chem., M. V. Lomonosov Moscow State Univ., Moscow, 119899, USSR  
 SO Inorg. Chim. Acta (1990), 169(1), 109-18  
 CODEN: ICHAA3; ISSN: 0020-1693  
 DT Journal  
 LA English  
 OS CASREACT 113:132367  
 AB An interaction of copper(I) halides with tantalocene trihydride  $\text{Cp}'_2\text{TaH}_3$  led to adducts of 2:1 ( $\text{Cp} = \eta^5\text{-C}_5\text{H}_5$ ) or 1:1 ( $\text{Cp}' = \text{C}_5\text{H}_5\text{CMe}_3$ ) compn. Structures of complexes  $(\eta^5\text{-C}_5\text{H}_5)_2\text{TaH}[(\mu_2\text{-H})\text{Cu}(\mu_2\text{-I})_2\text{Cu}(\mu_2\text{-H})]_2\text{TaH}(\eta^5\text{-C}_5\text{H}_5)$  (I) and  $(\eta^5\text{-C}_5\text{H}_4\text{CMe})_2\text{TaH}(\mu_2\text{-H})_2\text{Cu}(\mu_2\text{-I})\text{Cu}(\mu_2\text{-H})_2\text{TaH}(\eta^5\text{-C}_5\text{H}_4\text{CMe})_2$  (II) were established by X-ray anal. In both complexes the  $\text{Cu}(\mu_2\text{-I})_2\text{Cu}$  moiety is bonded with tantalum atoms by one (I,  $\text{Ta}\cdots\text{Cu} = 2.788 \text{ \AA}$ ) or two (II,  $\text{Cu}\cdots\text{Cu} = 2.844 \text{ \AA}$ ) hydrogen bridges. The model of bonding of  $\text{LnCu}(\mu_2\text{-I})_2\text{CuLn}$  complexes has been proposed and the conditions of realization of the bond between transition metal atoms with a d10 electron shell are discussed. It is shown that the conditions of  $n = 2$  and bulky ligand L are essential but insufficient, e.g. the 1:1 adduct of Cu(I) with bulky phosphine  $\text{P}(\text{NMe}_2)_3$  is a tetramer  $[\text{Cu}(\mu_2\text{-I})\cdot\text{P}(\text{NMe}_2)_3]_4$  without Cu-Cu bonds.

L24 ANSWER 9 OF 26 CA COPYRIGHT 1999 ACS

AN 112:217133 CA

TI Crystal and molecular structure of

bis(tert-butylcyclopentadienyl)tantalum trihydride complex with zinc chloride  $[\eta^5\text{-C}_5\text{H}_4\text{Bu-tert}]_2\text{Ta}(\text{H})(\mu_2\text{-H})_2\text{ZnCl}(\mu_2\text{-Cl})_2$

AU Gun'ko, Yu. K.; Bel'skii, V. K.; Sizov, A. I.; Soloveichik, G. L.; Bulychiev, V. M.

CS Mosk. Gos. Univ., Moscow, USSR

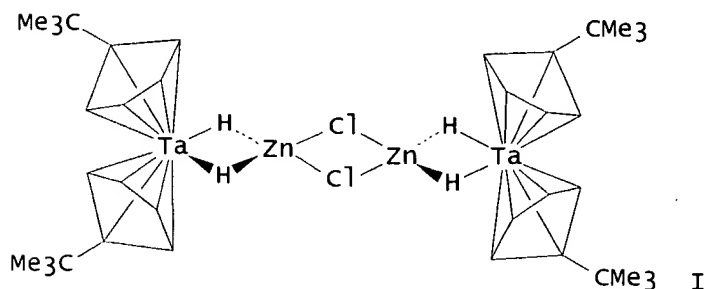
SO Metalloorg. Khim. (1989), 2(5), 1121-4

CODEN: MEKHEX

DT Journal

LA Russian

GI



AB Reaction of  $(\text{Me}_3\text{CC}_5\text{H}_4)_2\text{TaH}_3$  ( $\text{C}_5\text{H}_5 = \eta^5\text{-cyclopentadienyl}$ ) with  $\text{ZnCl}_2$  in THF-PhMe gave the bridged title compd. (I), the structure of which was detd. by x-ray crystallog.

L24 ANSWER 10 OF 26 CA COPYRIGHT 1999 ACS

AN 112:119088 CA

TI Hydride abstraction. The reaction of

[bis(diphenylphosphino)ethane]carbon ylhaloiridium with bis(cyclopentadienyl)trihydridotantalum

AU Deutsch, Paul P.; Maguire, John A.; Jones, William D.; Eisenberg, Richard

CS Dep. Chem., Univ. Rochester, Rochester, NY, 14627, USA

SO Inorg. Chem. (1990), 29(4), 686-90

CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

OS CASREACT 112:119088

AB The reaction of  $\text{IrX}(\text{CO})(\text{dppe})$  ( $\text{X} = \text{Br}, \text{I}$ ,  $\text{dppe} = 1,2\text{-bis(diphenylphosphino)ethane}$ ) with  $\text{Cp}_2\text{TaH}_3$  ( $\text{Cp} = \eta^5\text{-cyclopentadienyl}$ ) is extremely rapid and forms  $\text{fac-IrH}_3(\text{CO})(\text{dppe})$  and  $\text{Cp}_2\text{TaX}$ , or  $\text{Cp}_2\text{TaXL}$  ( $\text{L} = \text{CO}, \text{C}_2\text{H}_4, \text{PrC.tplbond.CPr}$ ) in the presence of added L. Trapping and

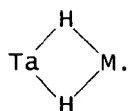
isotope-labeling expts. indicate that the reaction does not proceed through prodn. of free  $\text{IrH}_2\text{X}(\text{CO})(\text{dppe})$ ,  $[\text{IrH}(\text{CO})(\text{dppe})]$ , or  $[\text{Cp}_2\text{TaH}]$ .

The results are consistent with formation of unstable hydride and halide-bridged binuclear intermediates, in which transfer of all hydride and halide ligands occurs before fragmentation into mononuclear species.

L24 ANSWER 11 OF 26 CA COPYRIGHT 1999 ACS  
 AN 111:194955 CA  
 TI Comparative study on methods for synthesizing tantalocene trihydride  
 AU Zvukova, T. M.; Sizov, A. I.; Gun'ko, Yu. K.; Bulychev, B. M.; Soloveichik, G. L.  
 CS Inst. Khim. Fiz., Chernogolovka, USSR  
 SO Metalloorg. Khim. (1988), 1(5), 1179-83  
 CODEN: MEKHEX  
 DT Journal  
 LA Russian  
 AB Comparison of the known methods for prepn. of  $\text{Cp}_2\text{TaH}_3$  (I; .eta.5-cyclopentadienyl) showed that they either had poor reproducibility or were too labor-intensive. Modifications were developed for the two-stage (via  $\text{Cp}_2\text{TaCl}_2$ , with addnl. reducing agent NaCp) and direct [from  $\text{TaCl}_5$ , NaCp, and  $\text{NaAlH}_2(\text{OCH}_2\text{CH}_2\text{OMe})_2$ ] synthesis of I in  $\text{MeOCH}_2\text{CH}_2\text{OMe}$  in 20-30% yields.

L24 ANSWER 12 OF 26 CA COPYRIGHT 1999 ACS  
 AN 111:115407 CA  
 TI Bonding interactions between three adjacent hydrogen ligands.  
 Preparation and spectroscopic properties of the tantalum and niobium complexes  $[\text{Ta}(\text{H})_3(\text{C}_5\text{H}_5\text{-nRn})_2]$  ( $\text{R} = \text{SiMe}_3$ ,  $n = 1$  or  $2$ ) and  $[\text{Nb}(\text{H})_3(\text{C}_5\text{H}_5\text{-nRn})_2]$  [ $(n = 1, \text{R} = \text{Me}$  or  $\text{SiMe}_3; n = 2, \text{R} = \text{SiMe}_3)$ ]  
 AU Antinolo, Antonio; Chaudret, Bruno; Commenges, Gerard; Fajardo, Mariano; Jalon, Felix; Morris, Robert H.; Otero, Antonio; Schweltzer, Caroline T.  
 CS Univ. Alcala Henares, Madrid, Spain  
 SO J. Chem. Soc., Chem. Commun. (1988), (17), 1210-12  
 CODEN: JCCCAT; ISSN: 0022-4936  
 DT Journal  
 LA English  
 OS CASREACT 111:115407  
 AB The title complexes were prepd. in 60-70% yield by treating  $\text{MCl}_2(\text{C}_5\text{H}_5\text{-nRn})_2$  ( $\text{C}_5\text{H}_5 = \text{.eta.5-cyclopentadienyl}$ ; same R, n; M = Nb, Ta) with  $\text{NaAlH}_2(\text{OCH}_2\text{CH}_2\text{OMe})_2$  in PhMe. The Ta complexes are true hydrides, whereas the Nb complexes have bonding interactions among the three hydrogen atoms, as shown by short NMR T1 values and unusual couplings  $1\text{H}(\text{H},\text{H})$  which vary with temp. from less than 3 to about 100 Hz.

L24 ANSWER 13 OF 26 CA COPYRIGHT 1999 ACS  
 AN 110:173367 CA  
 TI Reactions of tantalocene trihydride  $(\text{.eta.5-C}_5\text{H}_5)_2\text{TaH}_3$  with second group metal halides. Crystal and molecular structure of  $(\text{.eta.5-C}_5\text{H}_5)_2\text{TaH}(\mu\text{-H})_2\text{ZnCl}_2 \cdot \text{C}_4\text{H}_8\text{O}$   
 AU Arkhireeva, T. M.; Bulychev, B. M.; Sokolova, T. A.; Soloveichik, G. L.; Belsky, V. K.; Boiko, G. N.  
 CS Chem. Dep., M. V. Lomonosov Moscow State Univ., Moscow, 119899, USSR  
 SO Inorg. Chim. Acta (1988), 141(2), 221-6  
 CODEN: ICHAA3; ISSN: 0020-1693  
 DT Journal  
 LA English  
 OS CASREACT 110:173367  
 GI



II

AB Interaction of Cp<sub>2</sub>TaH<sub>3</sub> (Cp = .eta.5-C<sub>5</sub>H<sub>5</sub>) with the Group II metal halides led to heterometallic complexes Cp<sub>2</sub>TaH<sub>3</sub>.cntdot.ZnCl<sub>2</sub>.cntdot.Et<sub>2</sub>O, Cp<sub>2</sub>TaH<sub>3</sub>.cntdot.ZnCl<sub>2</sub>.cntdot.THF (I), Cp<sub>2</sub>TaH<sub>3</sub>.cntdot.ZnI<sub>2</sub>.cntdot.Et<sub>2</sub>O, Cp<sub>2</sub>TaH<sub>3</sub>.cntdot.ZnI<sub>2</sub>.cntdot.THF, Cp<sub>2</sub>TaH<sub>3</sub>.cntdot.CdI<sub>2</sub>, and Cp<sub>2</sub>TaH<sub>3</sub>.cntdot.MgI<sub>2</sub>. According to IR and NMR data, the binding in soln. is accomplished via an ordinary hydrogen bridge Ta-H-M (M = Group II metal), whereas in the crystal state this is effected via a double hydrogen bridge, as in II. The interaction of Cp<sub>2</sub>TaH<sub>3</sub> with BeCl<sub>2</sub> and MgCl<sub>2</sub> in THF proceeds as a redox reaction to give Cp<sub>2</sub>TaCl<sub>2</sub> as one of the reaction products. Complex I has been studied by x-ray anal. The zinc atom in I possesses an unusual coordination no. equal to 5. The coordination polyhedron of the zinc atom is an essentially distorted trigonal bipyramid.

L24 ANSWER 14 OF 26 CA COPYRIGHT 1999 ACS

AN 109:6661 CA

TI Alpha- and beta-migratory insertion and elimination processes for alkyl complexes of permethylscandocene and permethyltantallocene

AU Parkin, G.; Bunel, E.; Burger, B. J.; Trimmer, M. S.; Van Asselt, A.; Bercaw, J. E.

CS Div. Chem. Chem. Eng., California Inst. Technol., Pasadena, CA, 91125, USA

SO J. Mol. Catal. (1987), 41(1-2), 21-39

CODEN: JMCADS; ISSN: 0304-5102

DT Journal

LA English

AB Beta-migratory insertion and elimination processes for alkyl derivs. of permethylscandocene, (.eta.5-C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>ScR, have been investigated.

Ethylene

is rapidly polymd. at -80.degree. by (.eta.5-C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>ScR (R = H, Me, Et, Pr, etc.) without the need for a co-catalyst. The relative rates of ethylene insertion into scandium-alkyl bonds and the propensity for .beta.-H elimination to afford olefin and (.eta.5-C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>ScH depend critically on the nature of R. With less sterically encumbered

scandocene

compds., e.g. [(eta.5-C<sub>5</sub>Me<sub>4</sub>)SiMe<sub>2</sub>(eta.5-C<sub>5</sub>Me<sub>4</sub>)]ScH, .alpha.-olefins are oligomerized selectively to the head-to-tail dimers, and catalytic cyclization of 1,5-hexadiene or 1,6-heptadiene to methylenecyclopentane

or

methylenecyclohexane is obsd. Both .alpha.- and .beta.-migratory insertion and elimination processes, which interconvert alkyl with alkylidene hydride or olefin hydride derivs. of permethyltantallocene

i.e.,

[(eta.5-C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>TaXR) .dblharw. (.eta.5-C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>Ta(:X)R (X = alkylidene, olefin; R = H, alkyl)], have been examd. For a complex with the alkyl substituent appended from a cyclopentadienyl ligand, [(eta.5-C<sub>5</sub>Me<sub>5</sub>)(eta.5, .eta.1-C<sub>5</sub>Me<sub>4</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>)Ta], the relative rates of .alpha.-H and .beta.-H elimination have been measured, and, significantly,

.alpha.-H

elimination is found to be 108 times faster than .beta.-H elimination at 100.degree.. The relative rates of the hydrogen and Me migrations to alkylidene, benzyne and olefin ligands have been detd. Related .alpha. and .beta. elimination processes have been examd. for some alkoxide, thiolate and amide derivs., [(eta.5-C<sub>5</sub>Me<sub>5</sub>)<sub>2</sub>TaYMe] (Y = O, S, NMe).

L24 ANSWER 15 OF 26 CA COPYRIGHT 1999 ACS

AN 107:217768 CA

TI Crystal and molecular structure of bimetallic complex of (.eta.5-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>TaH(.mu.2-H)<sub>2</sub>ZnCl<sub>2</sub>.C<sub>4</sub>H<sub>8</sub>O

AU Arkhireeva, T. M.; Bel'skii, V. K.; Bulychiev, B. M.; Soloveichik, G. L.

CS Otd. Inst. Khim. Fiz., Chernogolovka, USSR

SO Izv. Akad. Nauk SSSR, Ser. Khim. (1986), (12), 2819-21

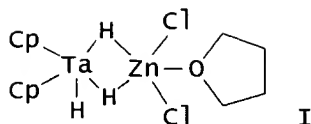
CODEN: IASKA6; ISSN: 0002-3353

DT Journal

LA Russian

OS CASREACT 107:217768

GI



AB The title complex (I, Cp = .eta.5-cyclopentadienyl) was prepd. by treating Cp2TaH3 with ZnCl2 in THF and its crystal and mol. structure detd.

L24 ANSWER 16 OF 26 CA COPYRIGHT 1999 ACS

AN 104:186564 CA

TI Bent-sandwich derivatives of tantalum bearing one or two pentamethylcyclopentadienyl ligands

AU Gibson, Vernon C.; Bercaw, John E.; Bruton, William J., Jr.; Sanner, Robert D.

CS Arthur Amos Noyes Lab. Chem. Phys., California Inst. Technol., Pasadena, CA, 91125, USA

SO Organometallics (1986), 5(5), 976-9

CODEN: ORGND7; ISSN: 0276-7333

DT Journal

LA English

OS CASREACT 104:186564

AB The compds. (.eta.5-C5Me5)2TaCl2 and (.eta.5-C5Me5)(.eta.5-C5H5)TaCl2 are prepd. in good yield by treatment of the trimethylphosphine adduct, (.eta.5-C5Me5)TaCl3(PMe3), with potassium pentamethylcyclopentadienide or sodium cyclopentadienide in refluxing toluene. Reaction of (.eta.5-C5Me5)2TaCl2 with Grignard reagents, RMgX (R = Et, Pr), affords the olefin complexes (.eta.5-C5Me5)2TaH(C2H3R') (R' = H, Me). Treatment of (.eta.5-C5Me5)2TaCl2 or (.eta.5-C5Me5)(.eta.5-C5H5)TaCl2 with LiAlH4

in di-Et ether, followed by aq. workup, gives (.eta.5-C5Me5)2TaH3 and (.eta.5-C5Me5)(.eta.5-C5H5)TaH3, resp., which react with two-electron donor ligands (L = CO, olefin) at elevated temp. to give (.eta.5-C5Me5)2TaH(L) and (.eta.5-C5Me5)(.eta.5-C5H5)TaH(L).

L24 ANSWER 17 OF 26 CA COPYRIGHT 1999 ACS

AN 103:178368 CA

TI Photochemistry of M(.eta.5-C5H5)2(H)CO and M(.eta.5-C5H5)2H3 (M = Nb, Ta) in low-temperature matrixes

AU Baynham, Robin F. G.; Chetwynd-Talbot, Jennifer; Grebenik, Peter; Perutz, Robin N.; Powell, Mark H. A.

CS Inorg. Chem. Lab., Oxford, UK

SO J. Organomet. Chem. (1985), 284(2), 229-42

CODEN: JORCAI; ISSN: 0022-328X

DT Journal

LA English

OS CASREACT 103:178368

AB Photolysis of MCp2H3 (M = Nb, Ta; Cp = .eta.5-cyclopentadienyl) in argon and nitrogen matrixes yields the 16-electron complexes MCp2H, previously (Klabunde, U.; Parshall, G., 1972) postulated as intermediates in the catalytic activation of aryl C-H bonds. The same complexes are generated by photolysis of MCp2(H)CO, together with small amts. of the 17-electron MCp2CO. In CO matrixes MCp2H3 is converted to MCp2(H)CO while further reaction of MCp2(H)CO yields MCp2CO and dicarbonyl products. The reactions were followed by IR and UV/VIS spectroscopy. The UV data on TaCp2H3 conflict with previously published (Foust, D., et al, 1982) soln. spectra.

L24 ANSWER 18 OF 26 CA COPYRIGHT 1999 ACS

AN 102:204067 CA

TI Carbon-hydrogen activation. Synthesis of silyl derivatives of niobocene and tantalocene hydrides, their H/D exchange reactions with benzene-d6

and the structure of Cp2Ta(H)2SiMe2Ph

AU Curtis, M. David; Bell, Larry G.; Butler, William M.

CS Dep. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA

SO Organometallics (1985), 4(4), 701-7

CODEN: ORGND7; ISSN: 0276-7333



DT Journal  
 LA English  
 OS CASREACT 102:204067  
 GI For diagram(s), see printed CA Issue.  
 AB Cp<sub>2</sub>MH<sub>3</sub> (M = Nb, Ta; Cp = cyclopentadienyl) reacted with PhMe<sub>2</sub>SiH to give Cp<sub>2</sub>M(H)<sub>2</sub>SiPhMe<sub>2</sub> (I). Cp<sub>2</sub>NbH<sub>3</sub> (II) reacted stoichiometrically with HSiMe<sub>2</sub>OSiMe<sub>3</sub> (III) to give partial conversion to Cp<sub>2</sub>Nb(H)<sub>2</sub>SiMe<sub>2</sub>OSiMe<sub>3</sub>, and catalyzed conversion of III to HSiMe<sub>2</sub>(OSiMe<sub>2</sub>)<sub>n</sub>OSiMe<sub>3</sub> (n = 1-3) and (Me<sub>3</sub>SiO)<sub>2</sub>SiMe<sub>2</sub>. II catalyzed H-D exchange between Et<sub>3</sub>SiH and C<sub>6</sub>D<sub>6</sub> and produced deuterated [Cp(μ-.eta.1,.eta.5-C<sub>5</sub>H<sub>4</sub>)HNb)]<sub>2</sub> as the major organometallic product. The x-ray crystal structure of I (M = Ta) (IV) showed the Ta-Si bond length was 2.651(4) Å. This is the first detn. of a Ta-Si bond length. Details of the <sup>1</sup>H NMR and the <sup>93</sup>Nb NMR of II were also reported.

L24 ANSWER 19 OF 26 CA COPYRIGHT 1999 ACS

AN 100:102730 CA  
 TI Olefin isomerization  
 IN Johnson, Thomas H.  
 PA Shell Oil Co., USA  
 SO U.S., 5 pp.  
 CODEN: USXXAM

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4423276	A	19831227	US 82-444755	19821126
AB	.alpha.-Olefins (I) are prepd. by isomerization of non-terminal olefins in				

an inert solvent using Ta complexes with cyclopentadiene (optionally alkyl-substituted). I form complexes with the catalyst which are decompd., with regeneration of the catalyst, by treatment with O<sub>2</sub>, CO, etc. I are then sepd. by distn. Thus, cis- and trans-MeCH:CHMe (45:55) in THF were treated with 10 mg trihydrobis(.eta.5-cyclopentadienyl)tantalum and heated 48 h at 100.degree. to give 11% conversion to EtCH:CH<sub>2</sub>. The catalyst also isomerizes trans- to cis-olefins.

L24 ANSWER 20 OF 26 CA COPYRIGHT 1999 ACS

AN 98:179536 CA  
 TI Substituted bis(cyclopentadienyl)tantalum complexes; synthesis and reactivity of dichlorides, tri- and monohydrides  
 AU Leblanc, Jean Claude; Reynoud, Jean Francois; Moise, Claude  
 CS Lab. Synth. Electrosynth., Fac. Sci., Dijon, 21100, Fr.  
 SO C. R. Seances Acad. Sci., Ser. 2 (1982), 295(8), 755-7  
 CODEN: CRSUDO

DT Journal  
 LA French

GI For diagram(s), see printed CA Issue.

AB Treating Ta dichlorides I (R = CMe<sub>3</sub>, SiMe<sub>3</sub>, CMe<sub>2</sub>Ph, CHMePh) with Na[AlH<sub>2</sub>(OCH<sub>2</sub>CH<sub>2</sub>OMe)<sub>2</sub>] gave the trihydrides II (same R). Carbonylation of II gave the monohydrides III (R = CMe<sub>3</sub>, SiMe<sub>3</sub>). Meso and racemic isomers of I and II (R = CHMePh) are obsd.

L24 ANSWER 21 OF 26 CA COPYRIGHT 1999 ACS

AN 94:84242 CA  
 TI Mono- and bis-.eta.-cyclopentadienyl derivatives of niobium and tantalum: improved synthetic routes via trialkyl(cyclopentadienyl)tin reagents  
 AU Bunker, Mark J.; De Cian, Andre; Green, Malcolm L. H.; Moreau, Joel J.  
 E.; Sigantoria, Nauzer  
 CS Inorg. Chem. Dep., Univ. Oxford, Oxford, OX1 3QR, Engl.  
 SO J. Chem. Soc., Dalton Trans. (1980), (11), 2155-61  
 CODEN: JCDTBI; ISSN: 0300-9246

DT Journal  
 LA English

AB Reaction of MX<sub>5</sub> (M = Ta, Nb; X = Cl, Br) with SnBu<sub>3</sub>(.eta.-C<sub>5</sub>H<sub>4</sub>R) (C<sub>5</sub>H<sub>5</sub> = cyclopentadienyl; R = H, Me) gave MCl<sub>4</sub>(C<sub>5</sub>H<sub>4</sub>R), TaX<sub>2</sub>(.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>, and NbCl<sub>2</sub>(.eta.-C<sub>5</sub>H<sub>4</sub>Me)<sub>2</sub> in high yields. NbCl<sub>4</sub>(.eta.-C<sub>5</sub>H<sub>4</sub>Me) with MeCN, PhCN, P(OMe)<sub>3</sub>, and (Ph<sub>2</sub>PCH<sub>2</sub>)<sub>2</sub> (L) gave NbCl<sub>4</sub>(.eta.-C<sub>5</sub>H<sub>4</sub>Me)L. Ta(.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>H<sub>3</sub> and Ta(.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(L)<sub>2</sub> [(L)<sub>2</sub> = (SMe)<sub>2</sub>, PhCH<sub>2</sub>Cl] were prepd. from TaCl<sub>2</sub>(.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>. Partial hydrolysis of NbCl<sub>4</sub>(.eta.-C<sub>5</sub>H<sub>4</sub>Me) gave [NbCl<sub>3</sub>(.eta.-C<sub>5</sub>H<sub>4</sub>Me)(OH<sub>2</sub>)]<sub>2</sub>O. Redn. of NbCl<sub>4</sub>(.eta.-C<sub>5</sub>H<sub>5</sub>) with [AlEtCl<sub>2</sub>]<sub>2</sub> in the presence of (Ph<sub>2</sub>PCH<sub>2</sub>)<sub>2</sub> (L<sub>2</sub>) gave NbCl<sub>3</sub>(.eta.-C<sub>5</sub>H<sub>5</sub>)L<sub>2</sub>.PhMe, which reduced with Na amalgam in the presence of CO to give Nb(.eta.-C<sub>5</sub>H<sub>5</sub>)L<sub>2</sub>(CO)<sub>2</sub>, which, in turn, protonated in acid giving [Nb(.eta.-C<sub>5</sub>H<sub>5</sub>)L<sub>2</sub>(CO)<sub>2</sub>H][PF<sub>6</sub>]. NbBr<sub>3</sub>(.eta.-C<sub>5</sub>H<sub>5</sub>)L<sub>2</sub>.PhMe was prepd. from Nb(.eta.-C<sub>5</sub>H<sub>5</sub>)L<sub>2</sub>(CO)<sub>2</sub> and PhCH<sub>2</sub>Br, and [Pt[Ta(.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(SMe)<sub>2</sub>]<sub>2</sub>][PF<sub>6</sub>]<sub>2</sub> was prepd. from PtCl<sub>2</sub>(NPh)<sub>2</sub> and Ta(.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(SMe)<sub>2</sub>.

L24 ANSWER 22 OF 26 CA COPYRIGHT 1999 ACS

AN 90:55053 CA

TI New synthetic pathways in dicyclopentadienyltantalum chemistry

AU Green, Malcolm L. H.; Moreau, Joel J. E.

CS Inorg. Chem. Lab., Oxford, Engl.

SO J. Organomet. Chem. (1978), 161(2), C25-C26

CODEN: JORCAI; ISSN: 0022-328X

DT Journal

LA English

AB (.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>TaX<sub>2</sub> (.eta.-C<sub>5</sub>H<sub>5</sub> = cyclopentadienyl; X = Cl, Br) are prepd. in 80% yield by treating TaX<sub>5</sub> with (C<sub>5</sub>H<sub>5</sub>)SnBu<sub>3</sub>. (.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>TaH<sub>3</sub> (I) is formed in 42% yield from (.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>TaCl<sub>2</sub> and NaAlH<sub>2</sub>(OCH<sub>2</sub>CH<sub>2</sub>OMe)<sub>2</sub>. I with BuLi gives a Ta-Li deriv. which reacts with PhCH<sub>2</sub>Cl, giving (.eta.-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>Ta(CH<sub>2</sub>Ph)Cl.

L24 ANSWER 23 OF 26 CA COPYRIGHT 1999 ACS

AN 90:23204 CA

TI Synthesis and properties of dicyclopentadienyltantalum hydride olefin compounds

AU Klazinga, A. H.; Teuben, J. H.

CS Lab. Anorg. Chem., Rijksuniv. Groningen, Groningen, Neth.

SO J. Organomet. Chem. (1978), 157(4), 413-19

CODEN: JORCAI; ISSN: 0022-328X

DT Journal

LA English

AB Reactions of Cp<sub>2</sub>TaCl<sub>2</sub> (Cp = cyclopentadienyl) with RMgCl (R = Pr, Me<sub>2</sub>CH, Bu, Me<sub>2</sub>CHCH<sub>2</sub>, n-C<sub>5</sub>H<sub>11</sub> and cyclopentyl) give tantalum hydride .pi.-olefin complexes Cp<sub>2</sub>Ta(H)L (L = CH<sub>2</sub>:CHR<sub>1</sub>, R<sub>1</sub> = Me, Et, Pr; cyclopentene). Two isomers of Cp<sub>2</sub>Ta(H)(CH<sub>2</sub>:CHMe) were obtained. The complexes are useful starting materials for the synthesis of other tantalum hydride species, e.g. Cp<sub>2</sub>Ta(H)PEt<sub>3</sub> and Cp<sub>2</sub>TaH<sub>3</sub>.

L24 ANSWER 24 OF 26 CA COPYRIGHT 1999 ACS

AN 86:132657 CA

TI Neutron diffraction studies of transition metal hydride complexes

AU Koetzle, T. F.; Bau, R.

CS Brookhaven Natl. Lab., Upton, N. Y., USA

SO Report (1976), BNL-21470, 10 pp. Avail.: NTIS

From: ERDA Energy Res. Abstr. 1976, 1(12), Abstr. No. 26207

DT Report

LA English

AB Investigations of H<sub>3</sub>Ta(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub> (I) (C<sub>5</sub>H<sub>5</sub> = cyclopentadienyl), HW<sub>2</sub>(CO)<sub>9</sub>(NO) (II), and HW<sub>2</sub>(CO)<sub>8</sub>(NO)(P(OMe)<sub>3</sub>) (III) have been completed. Preliminary results are available for HFeCo<sub>3</sub>(CO)<sub>9</sub>[P(OMe)<sub>3</sub>]<sub>3</sub> (IV). This work,

together

with studies of HMo<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(CO)<sub>4</sub>(PMe<sub>2</sub>) (V) and [Et<sub>4</sub>N][Cr<sub>2</sub>(CO)<sub>10</sub>H] (VI)

led

to some general observations on the geometry and the nature of bonding in these compds. For example, in the structures of II and III, both of

which

have bent W-H-W linkages (< W-H-W in the range 125-130.degree.), there is conclusive evidence for the existence of a closed 3-center W-H-W bond

with

significant metal-metal interaction. Such is the case, because

extensions

of the axial W-C and W-N bonds trans to the hydride intersect at a point near the center of the W-H-W triangle. The geometry of V, which also contains a bent M-H-M bond, is consistent with that of II and III. Bridging M-H bonds in these 2nd- and 3rd-row hydrides range in length from 1.85 to 1.89 .ANG., compared to 1.75 .ANG. in the 1st-row polynuclear complex IV. For metals of corresponding rows, bridging M-H bonds are about 0.1 .ANG. longer than terminal bonds, which are classified as single covalent bonds.

L24 ANSWER 25 OF 26 CA COPYRIGHT 1999 ACS

AN 79:92349 CA

TI Lewis acidic metal alkyl-transition metal complex interactions. I. Niobium and tantalum hydrides

AU Tebbe, Fred N.

CS Exp. Stn., E. I. du Pont de Nemours and Co., Wilmington, Del., USA

SO J. Amer. Chem. Soc. (1973), 95(16), 5412-14

CODEN: JACSAT

DT Journal

LA English

AB Lewis acidic metal alkyls react with dicyclopentadienyl niobium and -tantalum hydrides to produce Lewis acid-Lewis base adducts or the products of alkane elimination from these adducts. Stable adducts isolated are (C5H5 = cyclopentadienyl, C5H4 = .mu.-cyclopentadienyl): [(C5H5)(C5H4)NbHAlEt3]2, (C5H5)2Nb(C2H4)HAlEt3, (C5H5)2Nb(CO)HAlEt3, (C5H5)2NbPMe3HAlEt3, and (C5H5)2TaH3AlEt3. Stable products of alkane evolution isolated are (C5H5)2NbH2AlEt2 and [(C5H5)2NbH2]2Zn. Et3Al inhibits insertion of ethylene into the metal hydride bond in (C5H5)2Nb(C2H4)HAlEt3.

L24 ANSWER 26 OF 26 CA COPYRIGHT 1999 ACS

AN 66:28900 CA

TI Dicyclopentadienyltantalum (and niobium) trihydrides

IN Wilkinson, Geoffrey

PA Ethyl Corp.

SO U.S., 5 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3288829		19661129		
PRAI	GB		19610119		
AB	The title compds. are useful as plating agents, fuel and oil additives, polymerization catalysts, and pesticides. E. g., 22 g. Na cyclopentadienide was dissolved in 420 g. tetrahydrofuran (THF), 15 g. NaBH4 was added, the resulting soln. cooled to -50.degree., 45 g. TaCl5 was added, the mixt. was refluxed under N 12 hrs., the THF was distd. off, and the solid residue sublimed under N in vacuo at 110-20.degree. to yield 70-80% dicyclopentadienyltantalum trihydride, cryst. solid stable in air for only a short time and sol. in benzene. Similarly prepd. was dicyclopentadienyl niobium trihydride.				

=> d 123 bib abs

L23 ANSWER 1 OF 1 CA COPYRIGHT 1999 ACS

AN 118:259466 CA

TI Low-temperature chemical vapor deposition or laser photodeposition of metals on substrates by using organometallic compounds

IN Hicks, Robert F.; Kaesz, Herbert D.; Xu, Dagiang

PA University of California, Berkeley, USA

SO U.S., 8 pp. Cont.-in-part of U.S. Ser. No. 260,799, abandoned.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5130172	A	19920714	US 89-428245	19891026 <--
PRAI	US 88-260799		19881021		
AB	Metals are deposited on Si or W substrates at .apprx.20- .ltoreq.190.degree. by using organometallic compd. LnMRm in presence of H. L in the compd. is H, ethylene, allyl, methylallyl, butadienyl, pentadienyl, cyclopentadienyl, methylcyclopentadienyl, cyclohexadienyl, hexadienyl, cycloheptatrienyl, or a deriv. of these compds. having .gtoreq.1 C5 alkyl side chain; M is a metal that can readily cycle between 2 oxidn. states and can catalyze hydrogenation of hydrocarbon ligands of the compd.; R is Me, Et, Pr, or Bu; and n and m are each a no. from 0 to the valence of the metal. The compd. is vaporized at .apprx.20- 100.degree.. M is selected from the group of metals having at. no. 22-29, 40-47, and 72-79 or 25-29, 42-47, and 74-79 or Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag, Au, and W.				

09/012,679

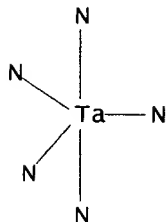
(FILE 'HOME' ENTERED AT 11:29:02 ON 15 APR 1999)

FILE 'REGISTRY' ENTERED AT 11:29:11 ON 15 APR 1999

L1 STRUCTURE UPLOADED  
L2 QUE L1

=> d l1

L1 HAS NO ANSWERS  
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l2

SAMPLE SEARCH INITIATED 11:29:38 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 32 TO ITERATE  
100.0% PROCESSED 32 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 301 TO 979  
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1

=> s l2 full

FULL SEARCH INITIATED 11:29:45 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 577 TO ITERATE  
100.0% PROCESSED 577 ITERATIONS 3 ANSWERS  
SEARCH TIME: 00.00.01

L4 3 SEA SSS FUL L1

=> fil ca

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	120.30	120.45

FILE 'CA' ENTERED AT 11:29:59 ON 15 APR 1999  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1967 - 10 Apr 1999 (19990410/ED) VOL 130 ISS 16

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s 14

L5 2 L4

=> d 1-2 bib abs

L5 ANSWER 1 OF 2 CA COPYRIGHT 1999 ACS  
AN 93:8233 CA  
TI A convenient preparation of metal pseudohalide compounds  
AU Andersen, Richard A.  
CS Chem. Dep., Univ. California, Berkeley, CA, 94720, USA  
SO Inorg. Nucl. Chem. Lett. (1980), 16(1), 31-2  
CODEN: INUCAF; ISSN: 0020-1650  
DT Journal  
LA English  
AB A reaction of  $[(\text{Me}_3\text{Si})_2\text{N}]_3\text{HfCl}$  with  $\text{Me}_3\text{SiX}$  gave  $[(\text{Me}_3\text{Si})_2\text{N}]_3\text{HfX}$  ( $\text{X} = \text{Br}, \text{I}, \text{N}_3, \text{CN}$ ), quant.  $[(\text{Me}_3\text{Si})_2\text{N}]_2\text{Ta}(\text{N}_3)_3$  was similarly prepd.

L5 ANSWER 2 OF 2 CA COPYRIGHT 1999 ACS  
AN 70:25323 CA  
TI Reactions between acetonitrile and dialkylamido-compounds of titanium, zirconium, and tantalum  
AU Bradley, Donald C.; Ganorkar, M. C.  
CS Queen Mary Coll., London, Engl.  
SO Chem. Ind. (London) (1968), (44), 1521-2  
CODEN: CHINAG  
DT Journal  
LA English  
AB  $\text{M}(\text{NMe}_2)_x$ , where  $\text{M} = \text{Ta}, \text{Zr}, \text{and Ti}$ , were treated with  $y$  moles of MeCN to give  $\text{M}[\text{N}:\text{C}(\text{Me})\text{NMe}_2]_y(\text{NMe}_2)^{x-y}$ . The ir spectra of these compds. showed a strong band in the 1577-87  $\text{cm}^{-1}$  region which was attributed to the NCN group of the dimethylaminoacetaldimino ligand, formed by insertion of MeCN in the  $\text{M}-\text{NMe}_2$  bond. The compds. prepd. and their characteristic ir bands were  $\text{Ti}[\text{N}:\text{C}(\text{Me})\text{NMe}_2](\text{NMe}_2)_3$  (I) 1580,  $\text{Ti}[\text{N}:\text{C}(\text{Me})\text{NMe}_2]_2(\text{NMe}_2)_2$  (II) 1577,  $\text{Zr}[\text{N}:\text{C}(\text{Me})\text{NMe}_2]_4$  (III) 1587,  $\text{Ta}[\text{N}:\text{C}(\text{Me})\text{NMe}_2](\text{NMe}_2)_4$  (IV) 1585  $\text{cm}^{-1}$ . Hydrolysis of these compds. gave  $\text{Me}_2\text{NH}$  and MeCN. Treatment of  $\text{Ti}(\text{NEt}_2)_4$  or  $\text{Zr}(\text{NEt}_2)_4$  with MeCN probably gave  $\text{Et}_2\text{NH}$  and  $\text{Ti}(\text{N}:\text{C}:\text{CH}_2)_2$  or  $\text{Zr}(\text{N}:\text{C}:\text{CH}_2)_2$  although their ir spectra had the characteristic bands at 1560 and 1587  $\text{cm}^{-1}$ , resp., assocd. with compds. I-IV.

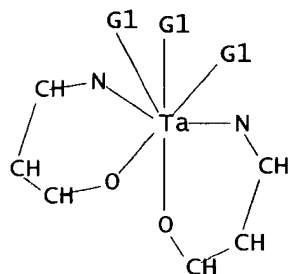
09/012,679

(FILE 'REGISTRY' ENTERED AT 11:41:12 ON 15 APR 1999)

L6 STRUCTURE UPLOADED  
L7 QUE L6

=> d 17

L7 HAS NO ANSWERS  
L6 STR



G1 H, Me, Et, n-Pr, i-Pr, n-Bu, i-Bu, s-Bu, t-Bu, Ph, CF3

Structure attributes must be viewed using STN Express query preparation.  
L7 QUE L6

=> s 17

SAMPLE SEARCH INITIATED 11:46:12 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE  
100.0% PROCESSED 5 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 5 TO 234  
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L6

=> s 17 full

FULL SEARCH INITIATED 11:46:45 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 80 TO ITERATE  
100.0% PROCESSED 80 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L9 0 SEA SSS FUL L6

09/012,679

(FILE 'HOME' ENTERED AT 16:04:37 ON 15 APR 1999)

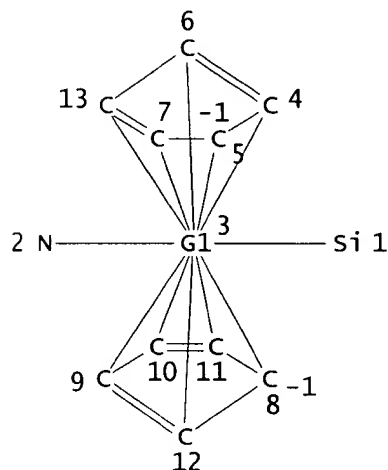
FILE 'REGISTRY' ENTERED AT 16:06:09 ON 15 APR 1999

E TITANOCENE/CN

L1 1 S E10  
L2 STR 1271-19-8  
L3 STR L2

=> d 13

L3 HAS NO ANSWERS  
L3 STR



VAR G1=TI/TA  
NODE ATTRIBUTES:  
CHARGE IS E-1 AT 5  
CHARGE IS E-1 AT 8  
DEFAULT MLEVEL IS ATOM  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

=> s 13

SAMPLE SEARCH INITIATED 16:08:13 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 55 TO ITERATE  
100.0% PROCESSED 55 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 656 TO 1544  
PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=> s 13 full



FULL SEARCH INITIATED 16:08:19 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 1027 TO ITERATE  
100.0% PROCESSED 1027 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

L5 0 SEA SSS FUL L3